VnmrJ 3.1 Industry-leading software for NMR spectrometers

Technical Overview

Key Benefits :

- Full integration of ChemPack
- An all-new simplified Sample-Centric workflow for setting up experiments
- Sample-Centric Data Management tools that logically index related data regard-less of instrument, date, or method of acquisition
- qNMR: a set of all-new Quantification tools
- ProShim : makes manual shimming a thing of the past
- Adaptive NMR: Avoid guessing and maximize the time-efficiency of your experiment
- Updated DOSY : more accurate and precise measurement of diffusion coefficients

Hardware supported by VnmrJ 3.1

Spectrometers

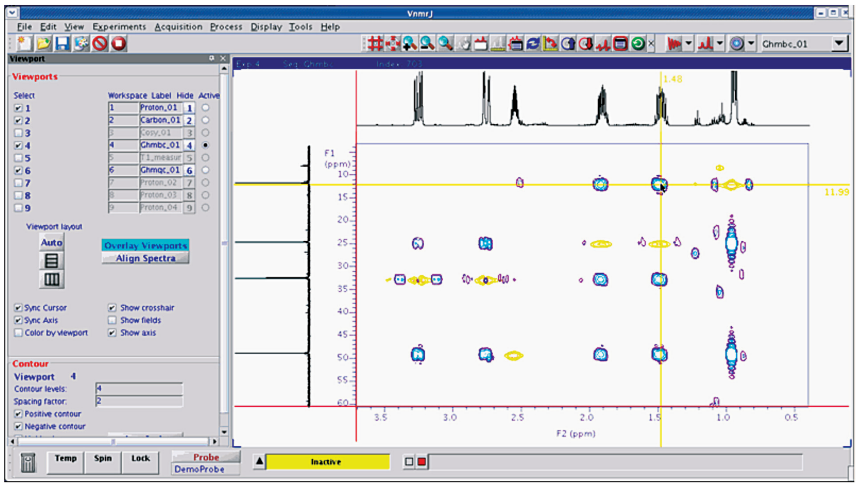
- Agilent DD2
- Agilent 400-MR DD2
- Varian VNMRS
- Varian 400-MR

Accessories

- 7600-AS (96 samples)
- 7510-AS (12 samples)
- SMS
- Carousel
- 7700-CS (Cold Probe chiller)
- E5025 Cryogen Monitor
- MAS Speed Controller
- Probes
- OneNMR Probe with ProTune-PZT
- All other liquids probes with or without ProTune
- Solids and Microimaging probes

Supported add-on packages

- DOSY for VnmrJ 3.x
- STARS
- Projection Reconstruction for BioPack



VnmrJ 3.1 is the latest release of host and data station software for Agilent's complete range of NMR & MRI spectrometers and accessories.

VnmrJ 3.1 covers:

- Small molecules in the solution state
- Static and spinning solid state spectroscopy
- BioNMR: protein, RNA and DNA solutions
- BioSolidsNMR: solid state biological NMR
- Tissues, beads, and gels
- LC/NMR/MS
- Imaging (horizontal)
- Microimaging (vertical)

Agilent Technologies

VnmrJ 3: a new generation of NMR host software

The complete queuing and acquisition engine in VnmrJ has been re-engineered by integrating ChemPack. This new infrastructure is available for all users, whether they are studying biomolecules or solid-state samples. Also coming from ChemPack as part of the integration is a cutting-edge pulse sequence library for scientists in the field of solution-state organic chemistry.

Data acquired with versions of VnmrJ prior to 3.0 are fully supported. A conversion tool is available to make older datasets sample-centric aware. With the same tool it is also possible to add pre-VnmrJ 3.0 data to a new or existing 'SampleQ'.

Workflow optimization has been a key feature of our development for this release. To that end, we have introduced the 'sample-centric' approach to setting up related experiments, acquiring data, and storing it in a logical form for easy retrieval when the time comes for processing and/or analysis.

Along with this version of VnmrJ 3.1, Agilent is introducing a new generation of DD2 NMR spectrometers. VnmrJ 3.1 fully supports these new spectrometers as well as the older Varian models : VNMRS ; and, 400MR.

A Sample-Centric unified workflow design

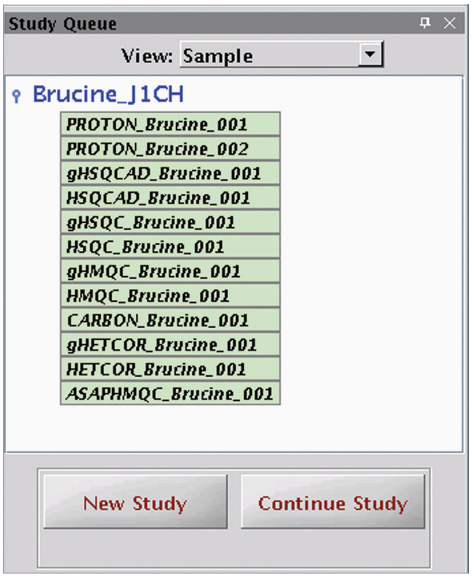
New for VnmrJ 3, the user can set up all desired experiments in a generic SampleQ using the familiar Experiment Selector & StudyQ interface without having to commit how the acquisition will take place. Only at the end does the user decide whether to send the list to the foreground or background (see the figure bottom right). If a sample changer is present, there will be a further choice to send the list to automation. All experimental events and results are identical regardless of foreground, background, or automation choice.

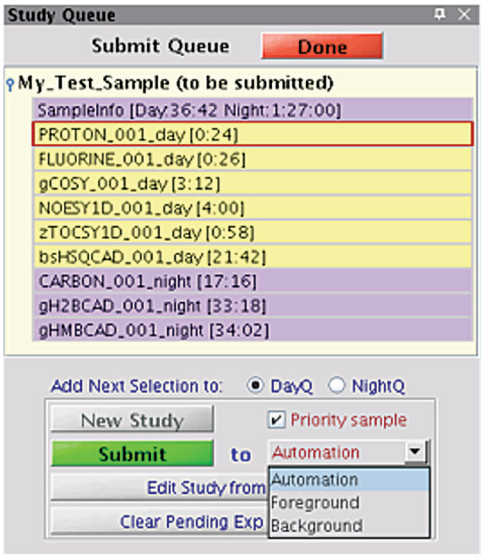
To achieve this simplicity, the StudyQ window now does double-duty: it is the familiar chronological view of what the spectrometer has queued up or has already acquired in a multi-user multi-sample environment; plus, it is now a 'Sample View' (see the figure bottom left) displaying a single SampleQ and hiding the chronological 'Spectrometer View.' One can flip back and forth at will, but it is the 'Sample View' that really brings the new unified workflow to life.

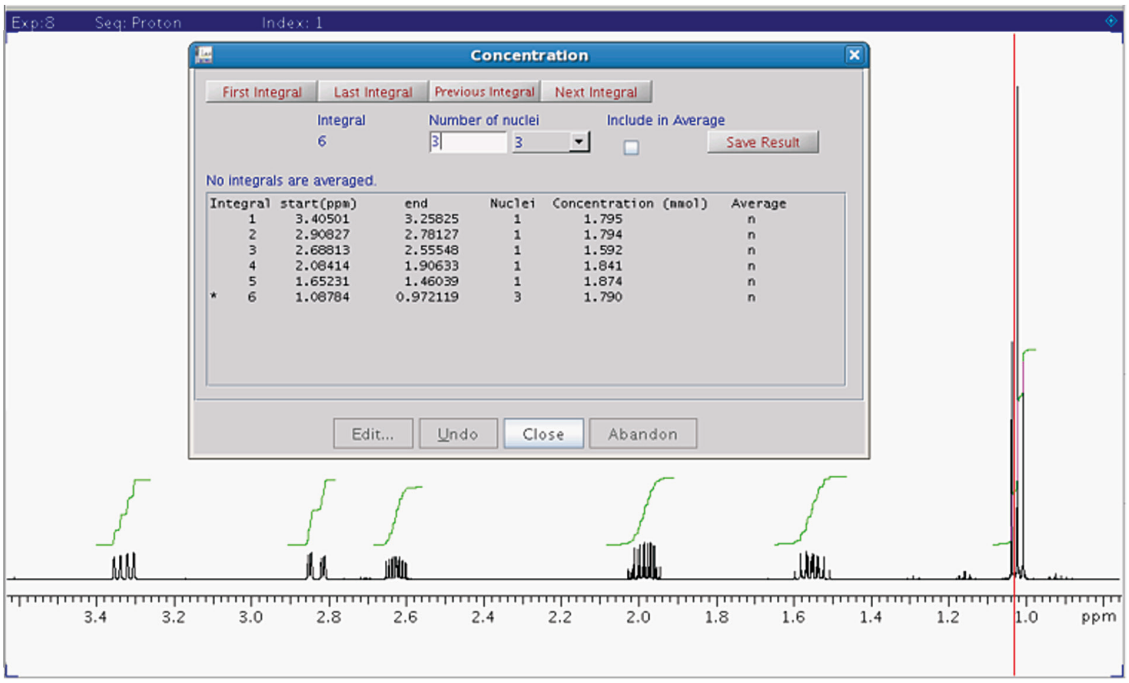
The immediate impact is tangible: all completed or pending experiments for a particular sample reside in the SampleQ, regardless of whether they were acquired in the foreground, background or automation; yesterday, today or tomorrow; DayQ or NightQ, and any combination of the above!

The SampleQ can be revisited in order to 'Continue Study' if more experiments are desired. All 'Continue Study' operations have the same flexibility to choose whether to send any new experiments to the foreground, background or automation, therefore it is possible to mix & match at the user's discretion based on need and/or availability of time or equipment. You can come back at any point and pick up where you left off.

And there is a bonus for those that have access to more than one spectrometer. As each SampleQ maintains its own mini-database containing file and content information, all the data in any one SampleQ can be stored in one place on a shared disk. Open a SampleQ in any instance of VnmrJ 3 and bring in the whole collection of data pertaining to your sample regardless of system, date, or method of acquisition. Drag and drop datasets into multiple Viewports for interactive analysis, all in one UI. VnmrJ 3 is truly sample-centric software.







'qNMR'

Quantification is an essential requirement for many NMR analyses. qNMR is a new method in VnmrJ 3 that delivers all the tools you need to accurately and precisely quantify your results quickly and easily. Crucially, it does not require any internal chemical standard or external signal injection, e.g. ERETIC. qNMR relies upon the superior stability and reproducibility of the Agilent DD2 console architecture that allows signals from distinct experiments to be used for calculations without any intrinsic normalization procedure, i.e. no need for a computer-generated synthetic signal to compensate for variability (e.g. QUANTAS). A one-time calibration of a compound of known concentration is all that is required, which is stored in the probe file for future use. All instrumental parameters and variables are seamlessly handled in the background, allowing the user to freely optimize experimental parameters for any acquisition without worrying about possible detrimental effects on the calculation.

Adaptive NMR

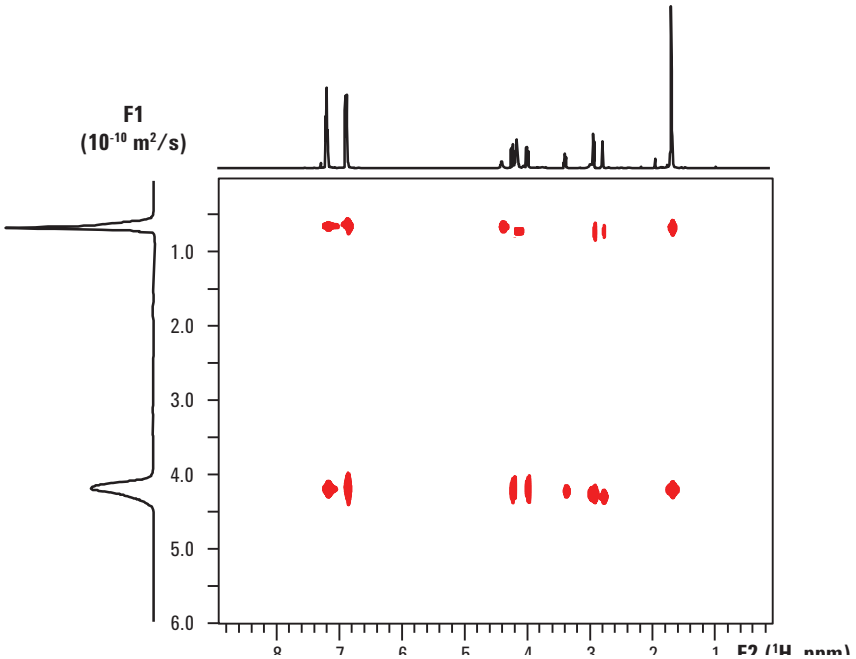
Have you ever wished that the NMR spectrometer could calculate the right number of transients that would ensure an acceptable signal-to-noise result for any experiment, and all you needed to supply was the concentration of your sample? Think how time-efficient that would be. Avoid having to re-acquire the data if you guessed low or wasting valuable magnet time if you guessed high. Adaptive NMR is a new tool in VnmrJ 3.1 that maximizes the time-efficiency of your experiments. By looking up a signal-to-noise threshold for an experiment in a user-configurable list, the software will intelligently and automatically set the number of transients necessary to achieve that threshold, or better. A one-time calibration of a Proton spectrum of known concentration, stored in the probe file, is all that is needed to enable Adaptive NMR. There are no limitations on the observe nucleus, pulse sequence complexity, or the dimensionality of the experiment. It is possible to adjust the acceptable threshold for any individual experiment, and the calculation will adapt to suit next time around. Adding a new experiment to the list or changing a threshold is as easy as editing a text file.

Enhanced DOSY application for VnmrJ 3

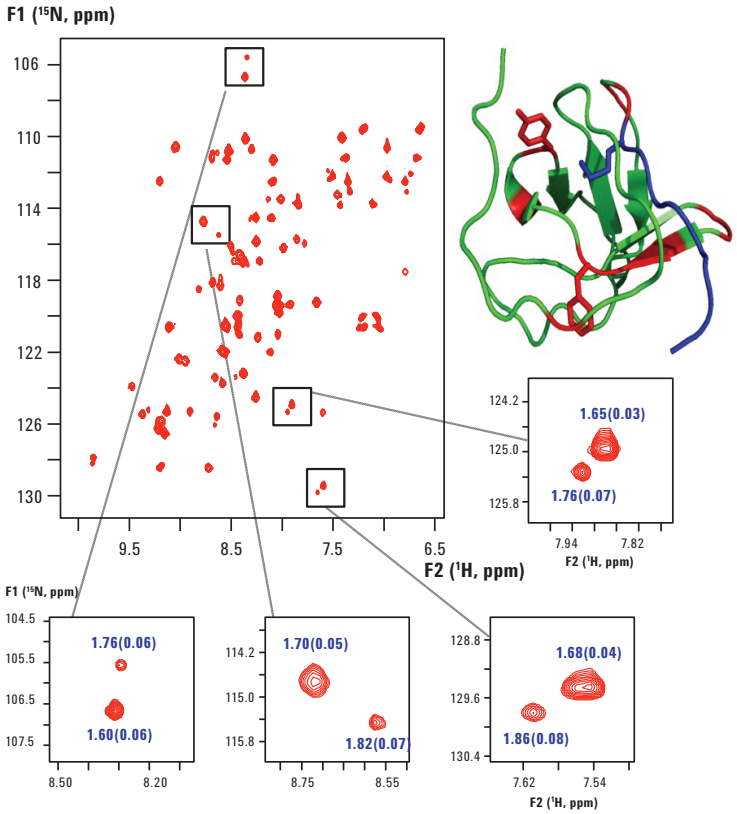
High-resolution Diffusion Ordered Spectroscopy (DOSY) is a very efficient tool for the mixture analysis of small and medium size molecules. Accurate determination of the diffusion coefficients may allow the separation of the NMR spectra of mixture components, or may serve as an experimental basis of predicting hydrodynamic radii, and therefore molecular weights. Diffusion data are also often used to monitor solution-state aggregation or binding between ligands and macromolecules.

The DOSY for VnmrJ 3.x add-on package is a greatly enhanced upgrade to our original DOSY software for diffusion coefficient measurements. It is licensed from Professor Gareth Morris, University of Manchester (UK), a pioneer and continuing leading contributor in the field of measurement of diffusion properties in NMR spectroscopy. Among the many improvements in the new package, the main additions are:

- Non-Uniform Gradient Calibration and Correction
- Multi-Exponential Fitting
  - CONTIN
  - SPLMOD
- Point-by-Point fitting
- Enhanced 3D DOSY processing
- Convection Compensation Experiments



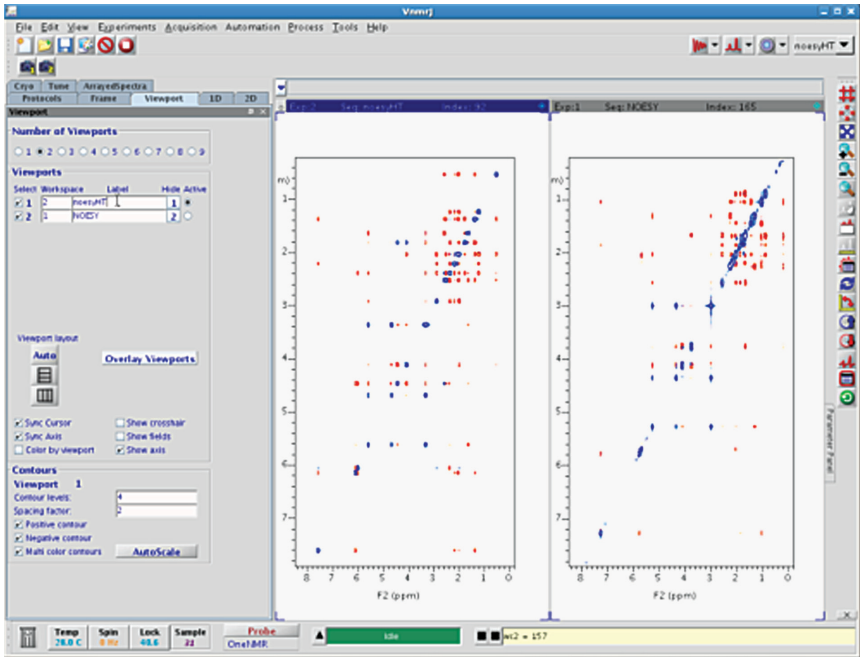
The 2D DOSY plot above shows the results of DOSY processing using multi-exponential fitting and NUG. On the top the high-resolution 1D spectrum ; on the side, the calculated "chromatogram".



15N-1H HMQC 3D DOSY spectrum of a protein together with four insets showing separated cross-peak pairs. The numbers in the insets represent the calculated D values with their statistical error in parenthesis.

More Fast Methods: A full suite of automated Hadamard experiments

Hadamard versions of the common experiments used by organic chemists are becoming more and more popular given that a time savings of an order of magnitude is possible (see the NOESY result below). Time is valuable, and when sufficient sample is available, Hadamard experiments can be the appropriate solution. In VnmrJ 3.1 we supply new Hadamard experiments, available in the Experiment Selector for easy access. It is also now possible to run all Hadamard experiments as a background task (sample changer optional).

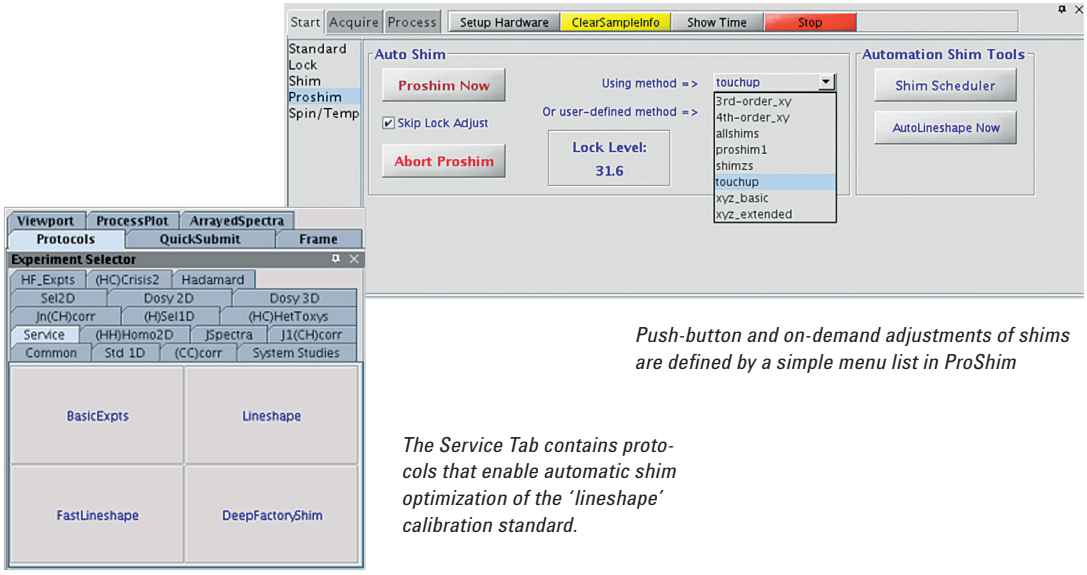


ProShim: make manual shimming a thing of the past.

VnmrJ 3.1 offers a new suite of tools that make the automated optimization of X-, Y-, and Z-axis shims easier. Control panels are provided (see figure below) that allow the operator to select from many included 'methods'. It is simple to create additional custom methods using a text editor.

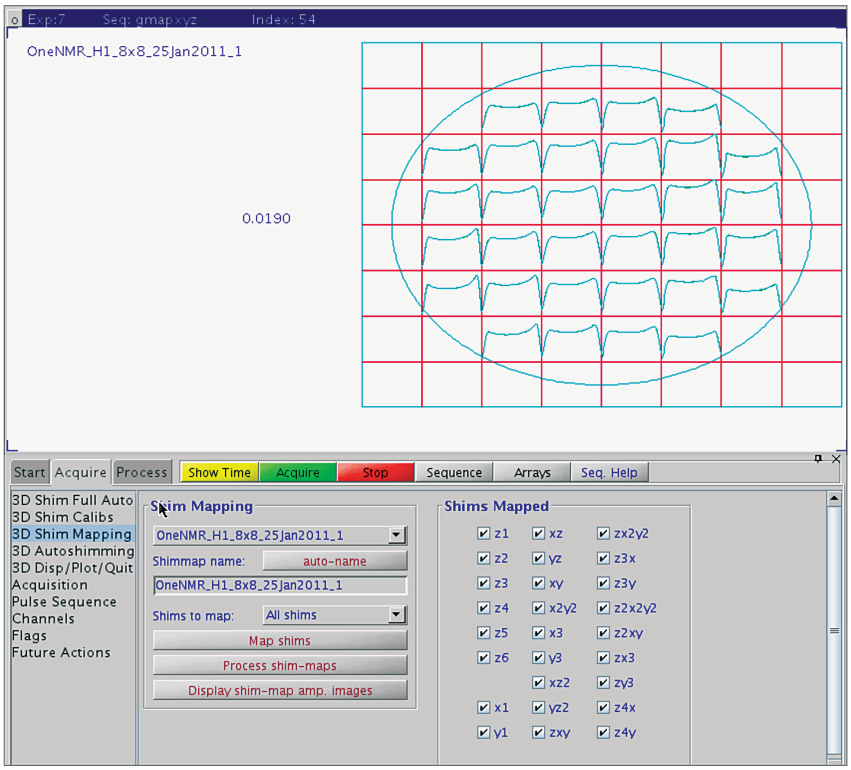
For those whose job it is to periodically check that the system is still performing at its optimum, but previously had to invest a significant amount of time and effort doing this task in a manual fashion, it is now possible to shim the 'lineshape' sample to within specification (see figure below).

And if you have a sample changer, this activity can also be scheduled for a time-slot of the operator's choosing, either one-time or on a regularly scheduled basis.



Push-button and on-demand adjustments of shims are defined by a simple menu list in ProShim

The Service Tab contains protocols that enable automatic shim optimization of the 'lineshape' calibration standard.



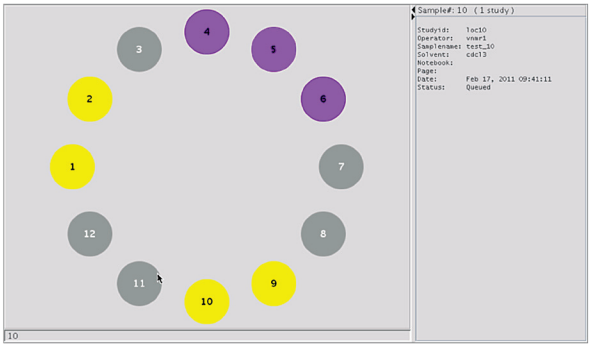
Installation and detailed magnet maintenance are made easy with the 3-D shimming application.

3D Gradient Shimming

3D gradient shimming is the preferred method for automatic setup of the complete set of starting shims in a new probe or magnet. The field mapping feature builds the table of files required for any gradient shimming method to function. Once the sample type has been selected from a menu, all calibrations, mapping steps, and shimming are carried out without further input from the operator. A variety of samples is supported and use is routine, even with probes that have no pulsed field gradient coils.

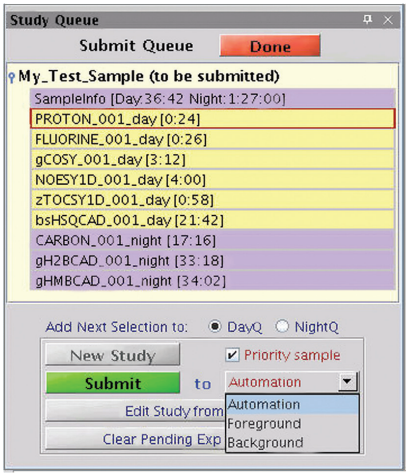
Automation Support: 7600-AS & 7510-AS Sample Changers

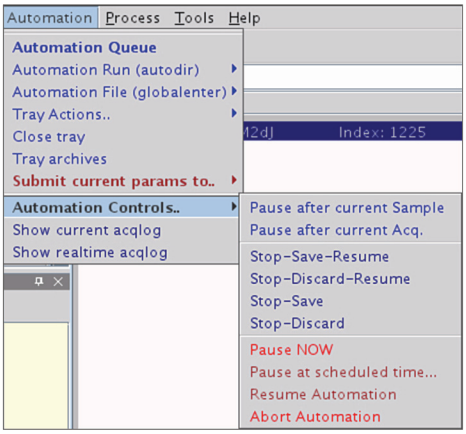
Full support for Agilent's 96-sample and 12-sample robotic sample changers is provided. The sample-centric design of VnmrJ 3.1 dovetails neatly into the common workflow for submitting experiments for acquisition. Learning a new way to use the software just because a sample changer is used is no longer necessary.

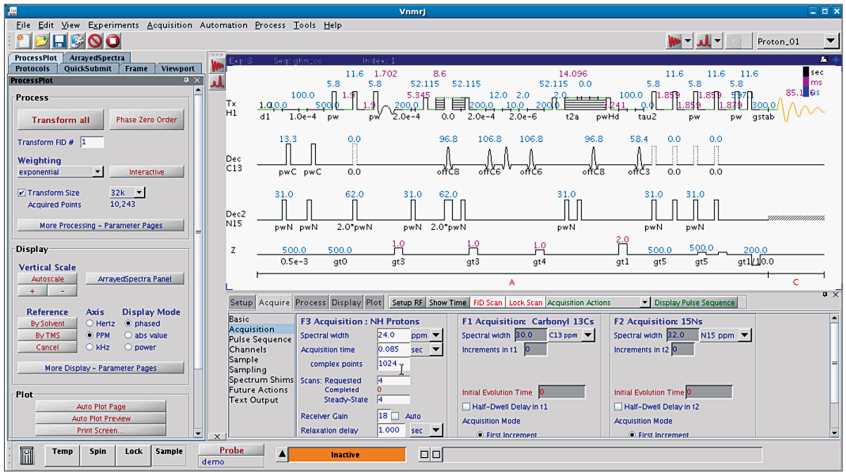


'Quick Submit' panel

The QuickSubmit panel can be used to set up and queue common experiments, with no need for the full-blown user interface. It works with or without a sample changer. QuickSubmit enables chemists to get in and out of the laboratory in the shortest possible time, while still allowing the local administrator to tailor and customize the list of available experiments and their parameters using the main set of panels and menus.







Precise and Flexible Control of Acquisition

VnmrJ 3 gives you much more control over the queue of experiments than ever before (see figure). Not only can one direct the queue to take the current experiment and save or discard it then resume with the next sample, one can pause the queue instantly or at a convenient time in the future, for example routine maintenance such as a cryogen fill. Log files are now also available from the menu in separate popup windows for convenient troubleshooting. Historical sample trays can be brought back on screen from the Tray Archives popup, and it is even possible to use an experiment from a previous tray as a template (aka a clone) for the current automation run.

BioPack

BioPack continues to be the world-leading software for acquiring NMR data for biomolecules. BioPack is now installed by default when loading VnmrJ 3.1 and can be enabled via the `Edit Applications' popup window. A full suite of pulse sequences are available to study proteins, RNA, or DNA complexes. There are experiments for backbone characterization, secondary and tertiary structure investigation, residual dipolar coupling measurement, relaxation time determination, and ligand binding.

There are now well over 350 distinct NMR pulse sequences to choose from, many of which have a multitude of options for further refinement of experimental requirements. BioPack continues to be updated via our web site on a regular and frequent basis, adding new experiments, new processing capabilities, as well as bug fixes.

Calibration is fully automatic, saving hours of manual experimentation optimizing selective pulses and water suppression parameters.

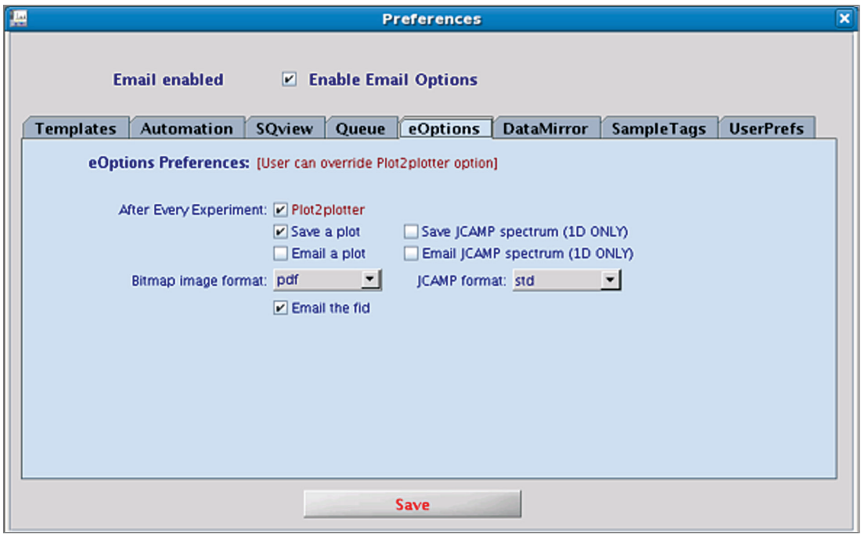
An extension is available, Projection Reconstruction for BioPack, that contains pulse sequences and processing tools for the new and exciting area of Projection Reconstruction, which enables faster acquisition of many experiments that traditionally take many hours to complete. Non-linear sampling acquisition schemes are also available to speed up data collection, with all the processing tools needed to produce and display a linearly-sampled computed dataset.

Preferences

VnmrJ 3.1 has taken a comprehensive new approach to gathering all of the options available to the user and presenting them in one convenient Preferences popup interface (see figure). Here one will find groups of options for setting up studies, sample changer configuration, queue control, output options, and data mirroring setup, amongst others.

Improved Output Options

In addition to the traditional paper output and electronic file (PDF, JPG, TIFF, etc.) VnmrJ 3.1 offers more parallel output capabilities: email a PDF ; plot a PDF ; save a PDF ; email raw data as a zipped attachment ; and, save a JCAMP.



For more information

Learn more:
www.agilent.com

Buy online:
www.agilent.com/chem/store

Find an Agilent customer center in your country:
www.agilent.com/chem/contactus

U.S. and Canada
1-800-227-9770
agilent_inquiries@agilent.com

Europe
info_agilent@agilent.com

Asia Pacific
adinquiry_aplsca@agilent.com

www.agilent.com

Product specifications and descriptions in this document are subject to change without notice.

© Agilent Technologies, Inc., 2011
Published in USA, April 8, 2011
Publication Number 5990-7611EN

Agilent Technologies